Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-Ethyl-4-{2-[1-(4-methylphenyl)ethylidene]hydrazinylidene}-3,4-dihydro-1*H*-2λ^6,1-benzothiazine-2,2-dione

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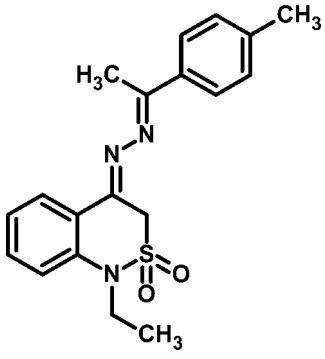
Received 27 December 2012; accepted 3 January 2013

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.048; wR factor = 0.139; data-to-parameter ratio = 15.7.

In the title compound, $C_{19}H_{21}N_3O_2S$, the dihedral angle between the aromatic rings is 6.7 (2)° and the C=N—N=C torsion angle is 178.0 (2)°. The conformation of the thiazine ring is an envelope, with the S atom displaced by 0.802 (2) Å from the mean plane of the other five atoms (r.m.s. deviation = 0.022 Å). In the crystal, molecules are linked by C—H···O interactions, generating $C(5)$ chains propagating in [010]. A weak C—H···π interaction is also observed.

Related literature

For the synthesis and biological activity of the title compound and related materials, see: Shafiq *et al.* (2011*a*). For further synthetic details, see: Shafiq *et al.* (2011*b*). For a related structure, see: Shafiq *et al.* (2013).



Experimental

Crystal data

$C_{19}H_{21}N_3O_2S$
M_r = 355.45
Monoclinic, $P2_1/n$
a = 15.9018 (10) Å
b = 7.3716 (4) Å
c = 16.8376 (10) Å
β = 111.644 (3)°
V = 1834.57 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 296 K
0.34 × 0.26 × 0.24 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.937, T_{max} = 0.955
14168 measured reflections
3597 independent reflections
2598 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.139
S = 1.02
3597 reflections
229 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*3 is the centroid of the C13–C18 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···O2^{i}	0.97	2.50	3.402 (4)	155
C9—H9A···*Cg*3^{ii}	0.97	2.67	3.613 (2)	165

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, y-1, z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 2012); software used to prepare material for publication: *SHELXL97*.

MS acknowledges the HEC Pakistan for providing a PhD fellowship and the University of Sargodha for the X-ray diffraction facility.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LD2091).

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supporting information

Acta Cryst. (2013). E**69**, o200 [doi:10.1107/S1600536813000202]

1-Ethyl-4-{2-[1-(4-methylphenyl)ethylidene]hydrazinylidene}-3,4-dihydro-1*H*-2λ^6,1-benzothiazine-2,2-dione

Muhammad Shafiq, M. Nawaz Tahir, William T. A. Harrison, Tanveer Hussain Bokhari and Muhammad Safder

S1. Comment

As a part of our ongoing studies of benzothiazine derivatives with potential biactivity (Shafiq *et al.*, 2011*a*,*b*), we now describe the synthesis and structure of the title compound, (I).

The dihedral angle between the C1–C6 and C13–C18 aromatic rings is 6.68 (15)° and the C10=N2—N3=C11 torsion angle is 177.98 (19)°. The conformation of the C1/C6/C9/C10/N1/S1 thiazine ring is an envelope, with the S atom displaced by 0.802 (2) Å from the mean plane of the other five atoms (r.m.s. deviation = 0.022 Å). A very similar conformation was observed in a related structure (Shafiq *et al.*, 2013). Atoms C7 and C8 in (I) are displaced from the mean plane of the thiazine ring by -0.416 (5) and 0.704 (6) Å, respectively.

In the crystal, the moelcules are linked by C—H···O interactions (Table 1) to generate C(5) chains propagating in the *b* axis direction. A weak C—H···π interaction to the C13—C18 ring also occurs (Table 1).

S2. Experimental

4-Hydrazinylidene-1-ethyl-3*H*-2?6,1-benzothiazine-2,2-dione (Shafiq *et al.*, 2011*b*) was reacted with *para*-methyl acetophenone according to literature procedure (Shafiq, *et al.*, 2011*a*). The product obtained was re-crystallized from ethyl acetate solution to yield yellow prisms.

S3. Refinement

The H atoms were placed in calculated positions (C—H = 0.93–0.97 Å) and refined as riding. The methyl group was allowed to rotate, but not to tip, to best fit the electron density. The constraint U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C) was applied.

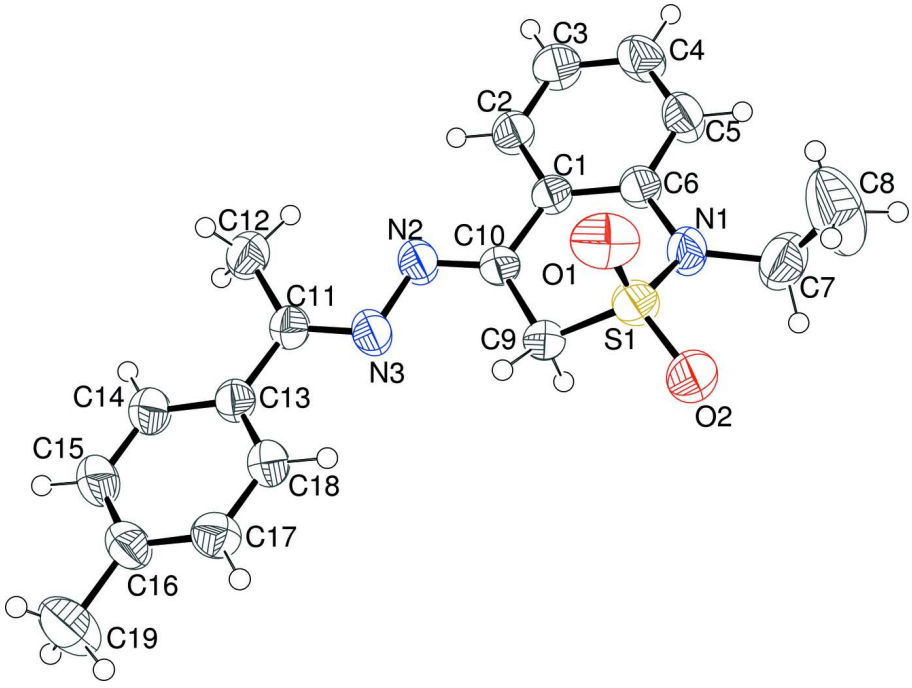

Figure 1

The molecular structure of (I), showing displacement ellipsoids at the 50% probability level.

1-Ethyl-4-{2-[1-(4-methylphenyl)ethylidene]hydrazinylidene}-3,4-dihydro- 1*H*-2λ^6,1-benzothiazine-2,2-dione

Crystal data

$C_{19}H_{21}N_3O_2S$
M_r = 355.45
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 15.9018 (10) Å
b = 7.3716 (4) Å
c = 16.8376 (10) Å
β = 111.644 (3)°
V = 1834.57 (19) Å^3
Z = 4
$F(000)$ = 752
D_x = 1.287 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 335 reflections
θ = 3.1–23.5°
μ = 0.19 mm^{-1}
T = 296 K
Prism, yellow
0.34 × 0.26 × 0.24 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.937, T_{max} = 0.955
14168 measured reflections
3597 independent reflections
2598 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 26.0°, θ_{min} = 1.5°
h = −19→18
k = −9→8
l = −18→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.139$
$S = 1.02$
3597 reflections
229 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0649P)^2 + 0.6783P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.
Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.53653 (13)	0.1072 (3)	0.23121 (12)	0.0401 (5)
C2	0.62165 (14)	0.1299 (3)	0.22572 (14)	0.0504 (6)
H2	0.6306	0.2260	0.1940	0.060*
C3	0.69200 (16)	0.0146 (4)	0.26570 (16)	0.0610 (7)
H3	0.7478	0.0324	0.2609	0.073*
C4	0.67962 (16)	−0.1279 (4)	0.31306 (17)	0.0629 (7)
H4	0.7274	−0.2057	0.3411	0.076*
C5	0.59694 (17)	−0.1552 (3)	0.31882 (16)	0.0609 (7)
H5	0.5891	−0.2528	0.3504	0.073*
C6	0.52430 (14)	−0.0399 (3)	0.27836 (14)	0.0460 (5)
C7	0.4152 (2)	−0.2572 (4)	0.3072 (2)	0.0795 (9)
H7A	0.3511	−0.2787	0.2768	0.095*
H7B	0.4483	−0.3488	0.2894	0.095*
C8	0.4360 (3)	−0.2746 (6)	0.3986 (3)	0.1315 (16)
H8A	0.4972	−0.2366	0.4293	0.197*
H8B	0.4290	−0.3989	0.4121	0.197*
H8C	0.3954	−0.1999	0.4147	0.197*
C9	0.37033 (14)	0.2050 (3)	0.18892 (14)	0.0478 (5)
H9A	0.3372	0.1275	0.1410	0.057*
H9B	0.3380	0.3191	0.1820	0.057*
C10	0.46398 (13)	0.2394 (3)	0.18915 (12)	0.0411 (5)
C11	0.43384 (14)	0.6397 (3)	0.08403 (13)	0.0451 (5)
C12	0.52607 (16)	0.6781 (3)	0.08357 (17)	0.0603 (6)
H12A	0.5486	0.7891	0.1138	0.090*
H12B	0.5226	0.6896	0.0257	0.090*

H12C	0.5661	0.5804	0.1110	0.090*
C13	0.36016 (14)	0.7729 (3)	0.04561 (13)	0.0443 (5)
C14	0.36872 (17)	0.9137 (3)	−0.00555 (15)	0.0558 (6)
H14	0.4221	0.9255	−0.0157	0.067*
C15	0.30017 (17)	1.0357 (4)	−0.04138 (15)	0.0620 (7)
H15	0.3081	1.1287	−0.0753	0.074*
C16	0.21992 (17)	1.0238 (3)	−0.02836 (14)	0.0553 (6)
C17	0.21100 (16)	0.8847 (3)	0.02377 (14)	0.0532 (6)
H17	0.1578	0.8748	0.0344	0.064*
C18	0.27955 (15)	0.7613 (3)	0.05990 (13)	0.0497 (5)
H18	0.2719	0.6691	0.0943	0.060*
C19	0.1445 (2)	1.1567 (5)	−0.0695 (2)	0.0903 (10)
H19A	0.1632	1.2757	−0.0467	0.135*
H19B	0.0920	1.1212	−0.0580	0.135*
H19C	0.1301	1.1580	−0.1302	0.135*
S1	0.37561 (4)	0.10183 (9)	0.28376 (4)	0.0544 (2)
O1	0.42132 (12)	0.2209 (3)	0.35183 (11)	0.0773 (6)
O2	0.28939 (11)	0.0333 (3)	0.27645 (13)	0.0771 (6)
N1	0.43901 (13)	−0.0742 (3)	0.28385 (14)	0.0600 (6)
N2	0.48467 (12)	0.3786 (3)	0.15443 (12)	0.0536 (5)
N3	0.41244 (13)	0.4972 (3)	0.11660 (12)	0.0546 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0382 (11)	0.0417 (12)	0.0417 (10)	0.0006 (9)	0.0160 (8)	−0.0016 (9)
C2	0.0434 (12)	0.0530 (14)	0.0597 (13)	0.0020 (10)	0.0248 (10)	0.0066 (11)
C3	0.0432 (13)	0.0687 (17)	0.0777 (16)	0.0086 (11)	0.0300 (12)	0.0084 (14)
C4	0.0482 (14)	0.0678 (17)	0.0753 (16)	0.0203 (12)	0.0257 (12)	0.0186 (13)
C5	0.0576 (15)	0.0597 (16)	0.0716 (15)	0.0152 (12)	0.0311 (12)	0.0236 (13)
C6	0.0406 (12)	0.0484 (13)	0.0526 (12)	0.0046 (9)	0.0214 (9)	0.0069 (10)
C7	0.0672 (18)	0.071 (2)	0.109 (2)	−0.0089 (14)	0.0431 (17)	0.0118 (17)
C8	0.167 (4)	0.132 (4)	0.138 (3)	0.049 (3)	0.105 (3)	0.063 (3)
C9	0.0376 (11)	0.0468 (13)	0.0555 (12)	0.0009 (9)	0.0132 (9)	0.0071 (10)
C10	0.0383 (11)	0.0425 (12)	0.0425 (10)	0.0002 (9)	0.0146 (9)	0.0005 (9)
C11	0.0472 (12)	0.0440 (13)	0.0459 (11)	−0.0017 (9)	0.0194 (9)	0.0027 (10)
C12	0.0517 (14)	0.0525 (15)	0.0792 (16)	−0.0029 (11)	0.0272 (12)	0.0070 (13)
C13	0.0477 (12)	0.0415 (12)	0.0425 (10)	−0.0024 (9)	0.0150 (9)	0.0020 (9)
C14	0.0538 (14)	0.0563 (15)	0.0589 (13)	−0.0025 (11)	0.0227 (11)	0.0149 (11)
C15	0.0665 (16)	0.0588 (16)	0.0601 (14)	0.0018 (12)	0.0226 (12)	0.0227 (12)
C16	0.0605 (15)	0.0522 (14)	0.0467 (12)	0.0083 (11)	0.0122 (11)	0.0093 (11)
C17	0.0489 (13)	0.0597 (15)	0.0511 (12)	0.0041 (11)	0.0186 (10)	0.0026 (11)
C18	0.0528 (13)	0.0472 (13)	0.0492 (12)	−0.0005 (10)	0.0191 (10)	0.0074 (10)
C19	0.083 (2)	0.099 (2)	0.089 (2)	0.0348 (18)	0.0322 (17)	0.0373 (19)
S1	0.0401 (3)	0.0653 (4)	0.0638 (4)	0.0066 (3)	0.0262 (3)	0.0137 (3)
O1	0.0671 (12)	0.1064 (16)	0.0636 (10)	0.0069 (10)	0.0302 (9)	−0.0119 (10)
O2	0.0449 (10)	0.0878 (13)	0.1101 (15)	0.0094 (9)	0.0422 (10)	0.0334 (11)
N1	0.0461 (11)	0.0570 (13)	0.0836 (14)	0.0062 (9)	0.0316 (10)	0.0266 (11)

N2	0.0456 (11)	0.0509 (12)	0.0679 (12)	0.0070 (8)	0.0251 (9)	0.0179 (10)
N3	0.0481 (11)	0.0499 (12)	0.0687 (12)	0.0076 (9)	0.0249 (9)	0.0193 (10)

Geometric parameters (Å, º)

C1—C6	1.399 (3)	C11—N3	1.287 (3)
C1—C2	1.400 (3)	C11—C13	1.482 (3)
C1—C10	1.477 (3)	C11—C12	1.497 (3)
C2—C3	1.368 (3)	C12—H12A	0.9600
C2—H2	0.9300	C12—H12B	0.9600
C3—C4	1.376 (3)	C12—H12C	0.9600
C3—H3	0.9300	C13—C14	1.387 (3)
C4—C5	1.368 (3)	C13—C18	1.391 (3)
C4—H4	0.9300	C14—C15	1.370 (3)
C5—C6	1.393 (3)	C14—H14	0.9300
C5—H5	0.9300	C15—C16	1.375 (3)
C6—N1	1.416 (3)	C15—H15	0.9300
C7—C8	1.456 (5)	C16—C17	1.391 (3)
C7—N1	1.493 (3)	C16—C19	1.505 (3)
C7—H7A	0.9700	C17—C18	1.377 (3)
C7—H7B	0.9700	C17—H17	0.9300
C8—H8A	0.9600	C18—H18	0.9300
C8—H8B	0.9600	C19—H19A	0.9600
C8—H8C	0.9600	C19—H19B	0.9600
C9—C10	1.509 (3)	C19—H19C	0.9600
C9—S1	1.742 (2)	S1—O1	1.4135 (19)
C9—H9A	0.9700	S1—O2	1.4233 (17)
C9—H9B	0.9700	S1—N1	1.643 (2)
C10—N2	1.282 (3)	N2—N3	1.397 (2)
C6—C1—C2	118.04 (19)	C11—C12—H12A	109.5
C6—C1—C10	122.43 (18)	C11—C12—H12B	109.5
C2—C1—C10	119.52 (19)	H12A—C12—H12B	109.5
C3—C2—C1	121.9 (2)	C11—C12—H12C	109.5
C3—C2—H2	119.1	H12A—C12—H12C	109.5
C1—C2—H2	119.1	H12B—C12—H12C	109.5
C2—C3—C4	119.6 (2)	C14—C13—C18	117.4 (2)
C2—C3—H3	120.2	C14—C13—C11	121.6 (2)
C4—C3—H3	120.2	C18—C13—C11	120.97 (19)
C5—C4—C3	120.0 (2)	C15—C14—C13	121.4 (2)
C5—C4—H4	120.0	C15—C14—H14	119.3
C3—C4—H4	120.0	C13—C14—H14	119.3
C4—C5—C6	121.4 (2)	C14—C15—C16	121.5 (2)
C4—C5—H5	119.3	C14—C15—H15	119.3
C6—C5—H5	119.3	C16—C15—H15	119.3
C5—C6—C1	119.1 (2)	C15—C16—C17	117.7 (2)
C5—C6—N1	120.1 (2)	C15—C16—C19	120.9 (2)
C1—C6—N1	120.82 (18)	C17—C16—C19	121.4 (2)

C8—C7—N1	112.2 (3)	C18—C17—C16	121.2 (2)
C8—C7—H7A	109.2	C18—C17—H17	119.4
N1—C7—H7A	109.2	C16—C17—H17	119.4
C8—C7—H7B	109.2	C17—C18—C13	120.9 (2)
N1—C7—H7B	109.2	C17—C18—H18	119.6
H7A—C7—H7B	107.9	C13—C18—H18	119.6
C7—C8—H8A	109.5	C16—C19—H19A	109.5
C7—C8—H8B	109.5	C16—C19—H19B	109.5
H8A—C8—H8B	109.5	H19A—C19—H19B	109.5
C7—C8—H8C	109.5	C16—C19—H19C	109.5
H8A—C8—H8C	109.5	H19A—C19—H19C	109.5
H8B—C8—H8C	109.5	H19B—C19—H19C	109.5
C10—C9—S1	110.92 (14)	O1—S1—O2	118.78 (12)
C10—C9—H9A	109.5	O1—S1—N1	110.96 (11)
S1—C9—H9A	109.5	O2—S1—N1	106.91 (11)
C10—C9—H9B	109.5	O1—S1—C9	107.98 (12)
S1—C9—H9B	109.5	O2—S1—C9	110.88 (10)
H9A—C9—H9B	108.0	N1—S1—C9	99.65 (11)
N2—C10—C1	117.42 (19)	C6—N1—C7	121.4 (2)
N2—C10—C9	123.51 (19)	C6—N1—S1	117.47 (16)
C1—C10—C9	119.07 (18)	C7—N1—S1	119.90 (17)
N3—C11—C13	115.83 (19)	C10—N2—N3	113.76 (18)
N3—C11—C12	124.8 (2)	C11—N3—N2	113.78 (19)
C13—C11—C12	119.40 (19)		

C6—C1—C2—C3	−0.8 (3)	C15—C16—C17—C18	−1.1 (3)
C10—C1—C2—C3	177.9 (2)	C19—C16—C17—C18	178.7 (2)
C1—C2—C3—C4	−0.2 (4)	C16—C17—C18—C13	0.3 (3)
C2—C3—C4—C5	1.0 (4)	C14—C13—C18—C17	0.5 (3)
C3—C4—C5—C6	−0.8 (4)	C11—C13—C18—C17	−179.7 (2)
C4—C5—C6—C1	−0.3 (4)	C10—C9—S1—O1	61.17 (18)
C4—C5—C6—N1	178.5 (2)	C10—C9—S1—O2	−167.11 (16)
C2—C1—C6—C5	1.1 (3)	C10—C9—S1—N1	−54.73 (18)
C10—C1—C6—C5	−177.7 (2)	C5—C6—N1—C7	−19.6 (4)
C2—C1—C6—N1	−177.7 (2)	C1—C6—N1—C7	159.1 (2)
C10—C1—C6—N1	3.6 (3)	C5—C6—N1—S1	147.7 (2)
C6—C1—C10—N2	173.5 (2)	C1—C6—N1—S1	−33.5 (3)
C2—C1—C10—N2	−5.2 (3)	C8—C7—N1—C6	92.8 (3)
C6—C1—C10—C9	−6.5 (3)	C8—C7—N1—S1	−74.3 (3)
C2—C1—C10—C9	174.75 (19)	O1—S1—N1—C6	−57.8 (2)
S1—C9—C10—N2	−144.76 (19)	O2—S1—N1—C6	171.25 (17)
S1—C9—C10—C1	35.3 (2)	C9—S1—N1—C6	55.80 (19)
N3—C11—C13—C14	−167.5 (2)	O1—S1—N1—C7	109.8 (2)
C12—C11—C13—C14	13.1 (3)	O2—S1—N1—C7	−21.2 (2)
N3—C11—C13—C18	12.7 (3)	C9—S1—N1—C7	−136.6 (2)
C12—C11—C13—C18	−166.7 (2)	C1—C10—N2—N3	−179.62 (17)
C18—C13—C14—C15	−0.7 (3)	C9—C10—N2—N3	0.4 (3)
C11—C13—C14—C15	179.6 (2)	C13—C11—N3—N2	−178.06 (18)

C13—C14—C15—C16	−0.1 (4)	C12—C11—N3—N2	1.3 (3)
C14—C15—C16—C17	1.0 (4)	C10—N2—N3—C11	177.98 (19)
C14—C15—C16—C19	−178.8 (3)		

Hydrogen-bond geometry (Å, º)

Cg3 is the centroid of the C13–C18 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7*A*···O2^{i}	0.97	2.50	3.402 (4)	155
C9—H9*A*···*Cg*3^{ii}	0.97	2.67	3.613 (2)	165

Symmetry codes: (i) −*x*+1/2, *y*−1/2, −*z*+1/2; (ii) *x*, *y*−1, *z*.